
Final Report: Third Peer Review of the CMAQ Model

Submitted to:

**Community Modeling and Analysis System Center
Carolina Environmental Program
The University of North Carolina at Chapel Hill**

Submitted by:

Anantha Aiyyer

Daniel Cohan

Armistead Russell

William Stockwell

Saffet Tanrikulu

William Vizquete

James Wilczak

North Carolina State University

Rice University

Georgia Tech

Howard University

Bay Area Air Quality Management District

University of North Carolina at Chapel Hill

National Oceanic and Atmospheric Administration

February 20, 2007

Table of Contents

1. INTRODUCTION.....	1
2. MAJOR DEVELOPMENTS SINCE SECOND PEER REVIEW (MAY 2005).....	2
3. SPECIFIC RECOMMENDATIONS OF SECOND PEER REVIEW PANEL AND AMD RESPONSE.....	5
4. PANEL'S RESPONSE TO CHARGE QUESTIONS	8
4-1. Charge Question 1: What is the overall quality of the applied scientific research in the CMAQ modeling program?	8
4-2. Charge Question 2: What are the strengths and weaknesses of the science being used within the components of the CMAQ model development program?.....	8
4-3. Charge Question 3: What is the quality and relevance of the model applications and evaluations being conducted as part of the CMAQ modeling program?	13
4-4. Charge Question 4: What are your perceptions of the integration across different elements of the CMAQ modeling program (links between model development, applications, evaluation)? What is your perception of the usefulness of the CMAQ modeling program to the EPA, states, other customer needs and research community?	15
4-5. Charge Question 5: Are there modeling research areas that are not being addressed or are given insufficient attention within the CMAQ modeling program? Are there current areas of research emphasis that might be given lower priority or eliminated? For the resources available to the CMAQ modeling program, are they being used in an effective manner in terms of the choice and quality of research being conducted?	16
5. COMMENTS ON THE PEER REVIEW PROCESS	17
6. CONCLUSIONS.....	18
7. REFERENCES.....	20
8. APPENDIX. CHARGE AND AGENDA FOR THIRD CMAQ PEER REVIEW MEETING.....	21

1. INTRODUCTION

The CMAQ Model External Peer Review Panel that conducted its review in December 2006 provides this review report, a follow-on to the series of reports of the first and second CMAQ Model External Peer Review Panel (Amar et al., 2004; 2005). The Atmospheric Modeling Division (AMD) of the National Exposure Research Laboratory (NERL) develops operational modeling tools for use in policy and regulatory analyses from research grade air quality models. This assessment focused on the work done by the complement of 36 staff scientists within AMD. The 2006 Peer Review emphasized an assessment of the meteorological/physical/chemical process aspects of the CMAQ modeling program, as well as applications and evaluation of model performance. The review panel focussed its attention on the current community version of CMAQ, version 4.6, which was released in October 2006.

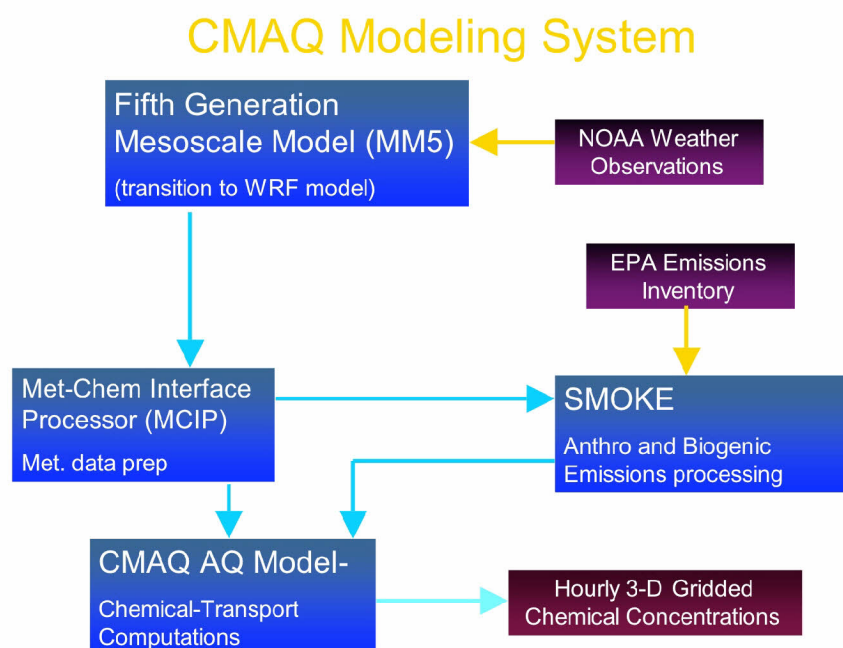
Within the context of the AMD's mission to develop air quality models for regulatory and operational purposes the panel was charged with evaluating the overall quality of the applied scientific research in the CMAQ Modeling Program. The panel evaluated the strengths and weaknesses of the science being used within the components of the CMAQ Model development program; the quality and relevance of the model applications and evaluations being conducted as part of the CMAQ Modeling Program; the integration of model development, applications, evaluation in the CMAQ Modeling Program; and the usefulness of the CMAQ Modeling Program to the EPA, states, other customer needs and research community. The panel evaluated the relevance of the AMD's modeling program elements in view of the resources available to the CMAQ Modeling Program. The panel was requested to identify relevant modeling research areas that are not being addressed or are given insufficient attention. The panel also identified current research areas that should be given lower priority or eliminated.

The report is written from the range of perspectives represented by the seven-member review panel: Anantha Aiyer, Daniel Cohan, Armistead Russell, William Stockwell, Saffet Tanrikulu, William Vizuite and James Wilczak. Panel members read a considerable volume of material on CMAQ provided by EPA and attended two days presentations on CMAQ by NOAA/EPA staff (see the Appendix for meeting agenda).

The panel finds that CMAQ modeling program continues to lead the state-of-the science. The overall breadth of the model development and research conducted by the CMAQ Modeling Program is unmatched by any other group worldwide. Model developers have done an outstanding job of incorporating new mechanisms, algorithms and data as they become available in the scientific literature, with appropriate consideration undertaken before incorporation and of developing new approaches when warranted. CMAQ is a modeling system that simulates a wide range of physical, chemical and biological processes (see figure below). There is a wide range in the level of scientific understanding of the processes modeled by CMAQ. There are a significant number of CMAQ processes and applications that are the target of active research by the AMD team and by many external groups worldwide. External groups use CMAQ for research and have developed very important new model code to extend its capabilities. Evaluation of CMAQ simulations by comparison with field data by the scientific community also points to needed improvements. The improvement in knowledge requires AMD to continually update CMAQ. Because it is both an operational and research model AMD needs to balance the timely release of improved versions against stability so that the model that can be used as a regulatory tool for the

evaluation of alternative control strategies. The addition of the new mission to support air quality forecasting places new requirements and constraints on AMD.

The review panel focused on the meteorological, physical and chemical processes of the CMAQ modeling program. The panel also evaluated some of AMD's model application and evaluation efforts along with its overall efforts to transfer research-grade air quality modeling techniques into operational tools. AMD has generally succeeded in its attempts to balance the demand for scientific completeness and rigor in the model with the need for computational efficiency as demanded of an operational tool used in applied research, regulatory analysis and air quality forecasting.



(Source: Presentation to Peer Review Panel by Jonathan Pleim, December 2006)

2. MAJOR DEVELOPMENTS SINCE SECOND EXTERNAL PEER REVIEW (MAY 2005)

The review panel was highly impressed by the depth and comprehensiveness of AMD's research and development of CMAQ. The panel feels that the CMAQ team has made significant progress since the last review (Amar et al., 2005). The team has managed to strike an appropriate balance between pursuing research and the development of regulatory modeling tools. They are performing excellent work. The committee was very impressed with clear understanding of the issues and their relative importance to their mission. The AMD's team has been very successful in finding an appropriate balance between the competing demands of scientific research quality and operational utility. They continue model developments on a number of fronts including the following efforts.

- The carbon bond gas-phase chemical mechanism has been updated to the new CB05 version mechanism. The new mechanism is more detailed than the earlier CB-IV with 52 chemical species and 156 reactions. The CB05 mechanism has about twice as many reactions as CB-IV but it is solved with the more efficient Euler Backward Iterative (EBI) solver. The CMAQ predicts summertime daily maximum 1-hr ozone concentrations that are about 9 % greater with CB05 than with CB-IV.
- Improvements to the heterogeneous chemistry have focused on N_2O_5 . The hydrolysis of N_2O_5 can be a significant loss of reactive nitrogen and an important source of nitrate. The N_2O_5 heterogeneous hydrolysis reaction probability is now a function of sulfate, nitrate, temperature and relative humidity. This change has led to a net decrease in the wintertime production of nitrate and to a slight increase in the summertime production.
- The treatment of aerosols has been updated to ISORROPIA, version 1.7. The new version of ISORROPIA includes a correction for the variation in activity coefficients with temperature. The relative humidity input from CMAQ to ISORROPIA was limited to 95%. Greater values resulted in the model forecasting extreme aerosol water content under humid conditions. The modification also reduced ammonium and nitrate aerosol concentrations.
- The numbers of gas phase hazardous air pollutants (HAPS) that can be modeled with SAPRC99 and CB05 mechanisms with CMAQ has been increased. The mercury modeling capability of CMAQv4.6 was updated. The diesel contributions to particulate matter and several toxic metals were added.
- A new planetary boundary layer (PBL) model that gives more realistic vertical profiles has been implemented in CMAQ, MM5 and WRF. The new Asymmetric Convective Model, version 2 (ACM2) replaces the previous ACM1. ACM2 combines non-local and local closure approaches. Large eddy simulations (LES) and 1-D tests show that it produces accurate simulation of vertical profiles and PBL heights. Tests with MM5 show good ground level performance and accurate PBL height evolution while WRF implementation is currently being tested.
- Other upgrades were made to the plume-in-grid module, the aerosol module and carbon apportionment. Sulfate tracking was revised to be consistent with CB05. The γ for N_2O_5 was added to the aerosol diagnostic file. A restart file that contains the last time step of the entire 4-D concentration array has been added and the parallel I/O code library has been updated.

There are a number of significant CMAQ improvements in progress that are expected to be completed during 2007 – 2008.

- The treatment of aerosols is being improved. A new secondary organic aerosol module is being developed. The aerosol module will include the biogenic precursors to aerosol formation, sesquiterpenes and isoprene. A new coarse particle chemistry module with treatment of the transfer of volatile inorganic material between the gas phase and the

coarse-particle mode is being developed. A new algorithm to moderate biogenic emissions to account for in-canopy deposition is being developed to substantially lower emission fluxes at night when turbulent transport is limited.

- An in-line photolysis module that calculates actinic flux in seven wavelength bands in the UV and visible is being implemented. The absorption cross-sections and quantum yields are being updated. The in-line photolysis module will include the effects of clouds, aerosol extinction and scattering, grid-specific surface albedo and meteorological and chemical profiles.
- The WRF/CHEM convective cloud model is being adapted for CMAQ in collaboration with Georg Grell (NOAA/OAR). The cloud mixing includes updraft, downdraft and compensating subsidence and the aqueous chemistry module in CMAQ will include a more detailed aqueous mechanism.
- AMD is developing methods to assimilate GOES derived clouds into CMAQ for retrospective simulations. The actinic flux used by CMAQ will be based on cloud parameters derived from GOES Visible and IR imagery.
- Other meteorological data assimilation developments include the implementation of GOES solar insolation data in MM5 and WRF and the development and implementation of soil moisture nudging in WRF.
- Methods for coupled synchronous meteorology and chemistry calculations are being developed. The system will allow chemical feedback to meteorology and aerosol feedback to the radiation model. The model will include integrated resolved-scale microphysics and aqueous chemistry. It will also include the indirect effects of aerosols on microphysics. This development will foster consistent air quality modeling between the meteorology and chemistry calculations in either a 2-way coupled or 1-way sequential execution. The prototype is anticipated in 2008.

The commitment of AMD to model evaluation is commendable. The modifications have undergone a preliminary evaluation of CMAQ's skill in simulating ozone and particulate matter for January and July with a horizontal resolution of 12 km and 14 vertical layers. The full evaluation will include simulations for January, April, July and October with horizontal resolutions of 12 and 36 km and 14 and 34 vertical layers. The panel recommends some reconsideration of its approach and goals. In particular, the current approach to uncertainty evaluation is unclear and more efforts should be devoted to dynamic evaluation.

We applaud the efforts of AMD to build the community of model developers (through maintenance of AMD staff and postdoctoral research fellows) and model users (in states, RPOs and the CMAS center). The Community Modeling and Analysis (CMAS) Center at UNC-CH/CEP continues to provide outreach. It provides client and customer support, training, help desk services, support for CMAQ model public releases and it provides web site and electronic resources. CMAS holds annual meetings for the national and scientific community and the most

recent CMAQ Annual Workshop was held on October 16-18, 2006 at the University of North Carolina at Chapel Hill with 200 participants.

We support the efforts of AMD to maintain the postdoctoral research fellowship program and believe that it continues to provide major rewards.

3. SPECIFIC RECOMMENDATIONS OF SECOND PEER REVIEW PANEL AND AMD RESPONSE

On the first morning of the review meeting, Dr. Ken Schere of AMD presented the following responses to the recommendations of the Second External Peer Review Panel (convened in May 2005):

- *Expanded use of post-docs should be encouraged; they have a positive impact on the program*
 - **Response:** We are actively participating in the EPA/NERL post-doc program, with 2 on the CMAQ team (several more openings are currently being advertised). We also seek post-docs in collaboration with ORISE and STC. Some of our post-docs have transitioned to EPA or NOAA positions on the CMAQ team.
- *Participate in meetings of the regulatory modeling community (e.g., RPO meetings) to obtain first-hand knowledge of how models are being applied and evaluated by these groups*
 - **Response:** CMAQ team members participated in RPO meteorology workgroup meetings in June 2005 and June 2006. We work closely with some states on science issues affecting their regulatory modeling. We work closely with EPA/OAQPS on use of CMAQ in rulemaking analyses, such as CAIR and CAMR.
- *Identified weakness: heterogeneous chemistry of N_2O_5*
 - **Response:** This has been a very active area of our research. The reaction probability (γ) of the N_2O_5 heterogeneous reaction to produce HNO_3 is now re-formulated in CMAQv4.6 to be a function of sulfate, nitrate, temperature and relative humidity (Evans and Jacob, 2005). We are working with Steve Brown (NOAA/ESRL) to incorporate latest information on measurements and chemistry of N_2O_5 from 2006 ICARTT field experiments.
- *Identified weakness: modal approach provides limited description of aerosol size distribution*
 - **Response:** In addition to the modal approach in CMAQ, we are working actively with CMAQ-UCD, containing a variation of the CalTech sectional approach. Current applications use 9-sections. This version may be released in the future, but currently has computational instabilities. CMAQ-MADRID, containing a sectional aerosol model, continues to be

upgraded by EPRI/AER and made available to the CMAQ community. We may yet add an ultrafine mode to CMAQ if there is interest and a scientific need.

- *Identified weakness: interactions between gases and coarse model aerosols*
 - Response: A current area of research is the dynamic interaction between fine and coarse model aerosols, including precursor gases (more on this later from Prakash Bhawe). We are also working with Thanos Nenes at Georgia Tech to extend the ISORROPIA thermodynamic module to include dust and crustal materials in the gas/aerosol partitioning mechanism.
- *Identified weakness: meteorologically-modulated fugitive dust emissions treatment*
 - Response: Current area of AQ forecast research is building on previous studies of D. Gillette and S. He.
- *Identified weakness: Re-emission of volatile and semi-volatile compounds*
 - Response: CMAQv4.6 has a simplistic parameterized Hg^0 re-emission, set to half of the deposited Hg^0 . We are actively working on building an emissions module in CMAQ, as part of the two-way interactive WRF-CMAQ work.
 - Will do biogenics, as well as Hg and NH_3 including re-emission based on meteorology.
- *Identified weakness: source apportionment tools*
 - Response: CMAQ model release now includes sulfate tracking and carbon apportionment tools. With recent hire from Georgia Tech, DDM will be actively pursued for source apportionment application.
- *Identified weakness: SOA chemistry*
 - Response: Major upgrade in SOA chemistry based on collaborative work with EPA/HEASD, Cal Tech (J. Seinfeld) and Univ. of East Anglia (S. Clegg) expected in next CMAQ release. Addition of isoprene and sesquiterpene pathways, among others.
- *Identified weakness: sub-grid vertical transport in deep convection*
 - Response: We are working with Georg Grell (NOAA/ESRL) to include his convective cloud parameterization scheme in CMAQ. We are working out some mass conservation issues with the scheme. Once working, we will add aqueous chemistry, chemical dynamics and wet deposition.
- *Identified weakness: inconsistent vegetation representation between BEIS and deposition models*
 - Response: Land use data for BEIS and M3Dry are based on same USGS 1-km database; implementation details differ. BELD database includes

USGS plus additional vegetation species data. We are working toward moving to higher-resolution National Land Cover Database (NLCD).

- *Identified weakness: weak measurement base for evaluation of CMAQ-Hg*
 - Response: Agree; measurements of Hg wet deposition are only consistent database available. We look to supplement these data with more intensive measurements from field studies.
- *Identified weakness: weak coupling with global chemical transport models*
 - Response: Initially GEOS-Chem was target of opportunity for providing mesoscale boundary conditions, through EPA/Harvard collaboration. Growing collaborations with NOAA/GFDL (AM2-Chem) and NOAA/NWS (GFS-Chem) will provide tighter link with global models. OAQPS has used hemispheric CMAQ domain; that is another option.
- *Plume-in-Grid (PinG) capability should be refined for more widespread use*
 - Response: Current PinG treatment for O₃ and PM_{2.5} is not being extended. Focus now is on hybrid models for plume treatments (CMAQ-AERMOD; CMAQ-HYSPLIT). We may return later to PinG or puff formulation as part of urban-scale studies and to treat in-plume Hg chemistry.
 - Line-source modeling in urban areas may also be a focus for sub-grid treatments in next few years.
- *Model performance criteria need to be developed based on comparing predicted changes with observed concentration changes due to changes in emissions*
 - Response: Agree; one of our focus areas in model evaluation is “dynamic” evaluation, which emphasizes this point. We are using the NOx SIP Call point source emissions reductions as a test for this dynamic evaluation procedure.
- *Improvements needed in clouds and precipitation*
 - Response: We have been collaborating with Univ. of Alabama-Huntsville on a data assimilation procedure using GOES satellite data for our retrospective simulations. Initially we will make operational the cloud and radiation information from GOES to better calculate chemical photolysis rates for CMAQ. We will also use surface solar insolation from GOES in MM5 and WRF meteorology simulations. Later we will use GOES skin temperature data assimilated into WRF for a better representation of the surface energy budget and soil moisture. We are also now improving our convective cloud parameterization scheme in the CMAQ model.
- *May be premature to move to WRF as a CMAQ met-driver model, as no four-dimensional data assimilation (FDDA) effort has been initiated*
 - Response: Since the May 2005 review, WRF has continued to be evaluated and refined by NCAR and many other groups. The latest

version, to be released in December 2006, will contain the initial capabilities for both analysis and observations nudging (FDDA). EPA/AMD helped support the collaboration between Penn State Univ. and NCAR to make this happen. We are now in the transition from MM5 to WRF and will be more actively using this model now that it contains FDDA.

- *Contributions to CMAQ from the larger developer community should be incorporated into the core model version.*
 - Response: We understand this desire and have heard this expressed many times. However, our resources do not allow us to make this happen for every contribution. Where we have active collaboration between AMD and outside scientists on a particular module, it is more likely to be brought into the core model (e.g., ISORROPIA, UCD sectional aerosols, DDM). Other modules have been supported by the external community and brought up to date with new CMAQ versions (e.g., MADRID aerosols supported by EPRI/AER).

4. PANEL'S RESPONSE TO CHARGE QUESTIONS

4-1. Charge Question 1: *What is the overall quality of the applied scientific research in the CMAQ Modeling Program?*

Overall quality: The CMAQ Modeling Program is conducting state-of-the-science model development and research whose overall breadth and quality is unmatched by any other group worldwide. Model developers have done an outstanding job of incorporating new mechanisms, algorithms and data as they become available in the scientific literature, with appropriate consideration undertaken before incorporation.

4-2. Charge Question 2: *What are the strengths and weaknesses of the science being used within the components of the CMAQ Model development program?*

Strengths and weaknesses of the science: The CMAQ team has done a commendable job in incorporating the best available science into the model with appropriate timing. Weaknesses of the science being used in CMAQ components mostly reflects weaknesses in current scientific understanding, including the following areas:

- a. Mercury chemistry
- b. How to effectively model cloud processes
- c. Secondary organic aerosol formation

Transition to the Weather Research and Forecast Model (WRF) (Priority High)

Efforts to develop the use of WRF as the meteorological driver for CMAQ are on track. Although the last review urged caution in this area, the ongoing development efforts appear to be warranted and successful. The work that is being done to transition to WRF merits strong support and should be accelerated. Although MM5 is not yet obsolete, it is clear that the meteorological modeling community is investing its resources in the development of WRF, not MM5. Comparisons of WRF (both ARW and NMM) and MM5 show similar skill. As time goes on the additional resources being focused on WRF will almost certainly increase its skill

and also add new functionality that MM5 will not have. To maintain CMAQ as a future viable air quality model it is important that a CMAQ-WRF interface be further developed. It is also important that the air quality community expedite the implementation of essential WRF features for air quality forecasting applications.

The two most critical aspects of improvements to WRF that are required for air quality simulations are the addition of nudging (both analysis and observations) and the addition of the ACM2 planetary boundary layer parameterizations. AMD has collaborated with Pennsylvania State University and the National Center for Atmospheric Research on the implementation of nudging and through their efforts it now appears that the next release of WRF-ARW will have basic nudging functionality. It is also hoped that progress is made towards incorporating surface nudging capability in addition to the basic nudging that has already been implemented. Importantly, AMD plans to continue this collaboration and make further advances to both analysis and observations nudging within WRF-ARW. AMD is also implementing the ACM2 PBL scheme in WRF (along with the PX LSM) that will be a welcome and important addition to the other PBL schemes available within WRF. In this regard, we also note that AMD plans to implement a snow model within the PX LSM to address a wintertime cold bias in both MM5 and WRF models and also incorporate an updated land use database. The panel believes that these developments are in the right direction.

Another critical research area that AMD is leading is implementation of satellite cloud information within the WRF/MM5/CMAQ modeling system. Because of the extreme sensitivity of ozone to cloud cover/solar radiation, the inability of meteorological models to get clouds correct (both in geographic location and opacity) has always been a weak part of the air quality modeling system. Assimilating a satellite-derived solar radiation field directly into CMAQ or WRF/MM5 is potentially a significant improvement for retrospective air quality simulations. The method currently used for the assimilation of cloud data is simply through the modification of the surface solar radiation, which is certainly the easiest way. However, AMD may also wish to consider assimilating the GOES cloud fields directly into the meteorological model by nudging the cloud liquid water field. Otherwise one might have the inconsistency of having clear sky radiation at the surface but vertical mixing and aqueous chemistry by convective clouds.

In addition to cloud information for correcting solar insolation in the model, satellite data can also be used during assimilation of soil moisture in the LSM. The development plan outlined by AMD includes a goal of nudging soil moisture in the PX LSM within the WRF using satellite derived skin temperature. This implementation in WRF should be accomplished along with the other changes to the LSM and PBL modules that are slated to be addressed.

It is also desirable that the CMAQ-MM5 interface still be available even after the full transition to WRF has been achieved. It is hoped that the code maintenance load will be small in order to retain the MM5 coupling option. The advantage of having different meteorological input options can be exploited for designing forecast applications using multi-model super-ensembles.

Planetary Boundary Layer (PBL) Model Development

Historically, vertical mixing in MM5 and other meteorological models has been parameterized using an eddy viscosity. By definition this mixing is down-gradient (often referred to as local mixing), from layers of higher potential temperature to lower potential temperature. However, in the convective planetary boundary layer large plumes can transport and mix heat across many layers of weakly stable stratification, i.e., up-gradient (often referred to as non-local mixing). To account for this counter-gradient mixing in the convective planetary boundary layer, the common solution has been to modify the vertical potential temperature gradient by subtracting off a small constant value in the planetary boundary layer, thereby changing the sign of the effective gradient. However, for chemical mixing it is problematic to apply the same gradient correction and the vertical mixing coefficients are all local by definition. This has been a long-standing, fundamental weakness of the CMAQ (and other) air quality modeling systems.

A different approach to parameterize vertical mixing in the convective planetary boundary layer has been to specify the eddy diffusion in terms of a complex matrix that determines the mixing between any two layers in the model and thereby incorporates both local and non-local mixing (sometimes referred to as transilient mixing). However, these matrices are difficult to determine and few (if any) chemistry models have used them. The new ACM2 planetary boundary layer parameterization scheme can be considered a truncated, or simplified form of the most general transilient mixing parameterization in that it includes mixing between adjacent layers but ignores mixing between non-adjacent layers other than that between the first layer and the layers above. However, it still maintains the basic feature of including both local and non-local mixing. Most importantly, the ACM2 modifies the eddy diffusion coefficient directly, so that a self-consistent mixing parameterization can be used for both meteorological and chemical variables.

The initial evaluation of the ACM2 scheme that was presented indicates that for meteorological variables (potential temperature, humidity and winds) it produces realistic vertical mean profiles that are in closer agreement with large eddy simulations than the previous ACM parameterization. Comparisons to wind-profiler derived planetary boundary layer depths shows reasonable agreement and comparison with a few ozonesondes also shows better capability in replicating the vertical ozone structure than the older ACM parameterization. We believe that the ACM2 parameterization will be seen as a major, step-function improvement in vertical mixing for CMAQ. Further testing of the ACM2 scheme should include more comparisons to measured PBL depths. Predicted ozone profiles could also be compared to ozone lidar profile data. This will complete the major development, in terms of transport, that can be accomplished in view of the present available science.

Chemical Mechanism Development

Presentations to the peer review panel included updates to the Carbon Bond chemical mechanism. The most recent version, CB05, was a USEPA sponsored project with principal investigators: Greg Yarwood, Gary Whitten and William Carter. The panel was satisfied with the improvements to the chemical mechanism including the 15 additional inorganic reactions and additional species for internal olefins, acetaldehyde, methane and ethane. Also promising was the addition of higher aldehyde, acylperoxy radical and peroxyacyl nitrate species to the mechanism. CB05 was expanded to include Hazardous Air pollutants (HAPS). This optional addition to the mechanism contains 28 gas phase species and 8 aerosol phase species. Also

added were four mercury reactions and dry/wet deposition rates. Improvements in the aerosol module included a new diagnostic output of PM_{2.5}, the addition of a RH cap in ISORROPIA and changes to N₂O₅ hydrolysis pathways.

The panel believes that the staff is working within a reasonable approximation of the best science in this area. It is also evident from the presentations that any new science updates presented in the literature are being critically reviewed and incorporated at a reasonable pace. We also agree with the following future work suggested by the presenters.

- Addition of the RACM2 chemical mechanism within CMAQ
- Inclusion of a surface heterogeneous HONO source to improve model performance
- Combine gas and aqueous phase chemistry modules
- Implement source apportionment for PM trace elements

The panel also believes that the following items require attention.

Nitrogen chemistry (Priority High)

Improvement of the treatment of the conversion of N₂O₅ to HNO₃ and the temperature dependencies of the processes affecting the transformation of nitrogen oxide to nitric acid in all phases is needed. Another important priority is to improve the performance of the model in predicting HONO. The panel recognizes that AMD has made extensive efforts in this area and it is possible that they may need to wait for further development of the science.

SOA formation (Priority High)

In-line with the Division's current efforts, greatest priority for the next release of CMAQ should be placed on improving the SOA module and cloud processes. The improvements should include production of SOA from biogenics and aromatics. Use an explicit chemical mechanism to guide protocols for developing a condensed mechanism. Use of process analysis and smog chambers is crucial for robust evaluation of mechanism performance. The panel notes that many of the current problems are due to gaps in fundamental knowledge so this will slow progress.

Mechanism Performance Evaluation (Priority High)

With the addition of the CB05 mechanism the USEPA also updated the process analysis algorithms to account for the expanded reaction set. This is an important update that allows for process-based evaluations of chemical dynamics. What is also needed is the quantification of the impact on pollutant predictions and response to precursor reductions. What would be the advantages and disadvantages of using different mechanisms?

Several detailed chemical mechanisms exist for the formation of SOA from reactive biogenic species (Lee et al. 2005; Leungsakul et al. 2005a,b; Tolocka et al. 2004). These mechanisms are in greater detail than the condensed chemical mechanisms currently used in the CMAQ aerosol modules. Although the sheer size of these mechanisms prohibits them in regulatory application, they remain an excellent resource to guide the process of mechanism reduction. With process analysis, relevant chemical pathways and cycles can be studied from a proposed reduced mechanism for SOA to that of the explicit mechanism. Thus, this data would provide evidence as to whether to add or delete chemical pathways. With confidence in the simulation of

chemical pathways attention can then be placed on the physical processes of aerosol partitioning, formation and transformation.

Cloud Chemistry and Physics (Priority High)

In CMAQ, scavenging and wet deposition for species relevant to cloud sulfur is calculated in the aqueous chemistry model; for other species, it is calculated through the use of a pollutant removal equation. Current CMAQ aqueous chemistry is based upon the RADM aqueous chemistry model. Both RADM and ACM cloud models have been incorporated into the CMAQ. Some comparisons against satellite data has been made. The committee supports the incorporation of the Grell Convective Cloud Model into the CMAQ and encourages conducting the suggested research to improve the estimation of pollutant removal from scavenging and wet deposition in CMAQ.

Aromatic chemistry (Priority Medium)

There is still great uncertainty in current chemical mechanisms' treatment of aromatic chemistry. This is especially relevant for urban areas where anthropogenic emissions of these species influence pollutant concentrations. A parameterized mechanism for aromatic chemistry may be useful until the current state of the science improves.

Scavenging and Wet Deposition (Priority Medium)

CMAQ uses a resistance model that includes aerodynamic resistance, laminar layer resistance and canopy resistance to estimate dry deposition. Pollutant pathways for stomata, leaf cuticle and ground are parameterized. Special attention was given to NH₃, Hg, toxic and aerosol depositions. While the resistance approach is a commonly used approach in air quality models, its accuracy has not been fully evaluated because of the lack of field data. Significant uncertainty may be introduced to model estimations due to uncertainties in the dry deposition algorithm. As planned, the use of the NLCD 2001 dataset may help refine some of the parameterizations and evaluation of the dry deposition algorithm.

In the short term, a study should be conducted to assess the overall uncertainty introduced to model forecasts due to uncertainty in the dry deposition. This can be done through model sensitivity simulations by varying key dry deposition parameters, comparing dry deposition against available data and comparing the resistance model used in CMAQ against other available dry deposition models. In the long run a comprehensive field campaign is needed to collect necessary data to fully evaluate and improve the dry deposition algorithm in CMAQ.

Multimedia Modeling (Priority Medium)

AMD is taking a prudent approach in its multimedia modeling of nitrogen to watersheds. While the multimedia modeling is not a central core function of CMAQ development, it has proven useful for building collaborations between AMD and other divisions of EPA. The multimedia modeling could also become important for evaluating the watershed impacts of policies to reduce nitrogen emissions, though caution should be taken given the current state of model performance.

The examination of Chesapeake Bay and other watersheds has been useful for highlighting strengths and weaknesses of CMAQ performance for wet and dry deposition of various nitrogen

compounds. AMD appears to be taking appropriate steps to address the identified biases in deposition rates.

HAP Chemistry (Priority Low)

Greater attention should be paid to photochemical reaction products of HAPs and their potential impact on human health. These reactions or intermediate species are currently not included in current chemical mechanisms.

Fine-Scale Modeling and Exposure – Model Limits (Priority Low)

The technique of using the CMAQ to address personal exposure is an interesting research direction. The decision to continue in this direction needs to be weighed with other research priorities. What are the limits of this approach and what are the uncertainties? What types of exposure and pollutants are the targets of this application?

4-3. Charge Question 3: *What is the quality and relevance of the model applications and evaluations being conducted as part of the CMAQ Modeling Program?*

AMD staff take the evaluation and application of CMAQ very seriously. Significant resources have been assigned by AMD to performance evaluation. We find the model applications and evaluations being conducted to be relevant and of high quality. The NOAA/EPA operational AQ forecasting program provides an additional test of CMAQ performance and AMD should continue to take full advantage of this opportunity. Some outstanding work is being done in applying and evaluating the CMAQ model, as demonstrated by the multitude of peer-reviewed articles published in quality scientific journals. However, much of the evaluation efforts have been devoted to operational evaluations of each year's release and the uncertainty evaluation approach has not been clearly articulated yet. The Program has made some headway toward dynamic evaluation through its efforts to examine CMAQ performance for capturing NO_x SIP Call impacts, but greater efforts are needed for dynamic and diagnostic evaluation. A thorough internal review of AMD's model evaluation efforts may be warranted to clearly define the objectives and goals and ensure that the approaches undertaken are appropriate and sufficient for meeting those goals.

Meteorological Model Evaluation (Priority High)

The motivations for performing comprehensive evaluation of the meteorological inputs stems from documented evidence of the sensitivity of air quality forecast to the state of the atmosphere. A better understanding of the sensitivity of the air quality forecasts will lead to a better description of the forecast uncertainty. Towards this end, it is desirable that the end users have access to a suite of routines that can be readily used to compute various metrics related to forecast evaluation. In this regard, the overall goals enumerated under the Atmospheric Model Evaluation Tool (AMET) project appear to be in the right direction.

One of the key features of the AMET is its coupling with the open source statistical analysis package "R". This will allow users to take full advantage of a powerful set of analysis tools. The choice of the model-matching database, MySQL, is also an apt one. In order to take full advantage of this capability, the user community will benefit from any simplification in the installation process of the AMET software system, given the various dependencies that must be preinstalled.

It is desirable that AMET's functionality will be expanded to also include non-standard data sources including satellite derived fields. AMET should be adapted to also cater to ensemble based modeling. Furthermore, there should be avenues to incorporate user developed analysis tools into AMET.

Apart from the technical aspects of model evaluation that fall under the purview of AMET development, it is also desirable that in house evaluations within AMD emphasize statistically rigorous techniques while performing intercomparisons. Sensitivity results should be accompanied by tests of significance of the patterns of anomalies or correlation. In order to obtain better insight into physical mechanisms underlying uncertainties in the model forecasts, metrics linking sensitivity of the air quality forecasts to the uncertainties in the meteorological inputs should also be developed.

Greater attention to model evaluation and analysis (Priority High)

To ensure that model evaluation matches needs of the user community we recommend a workshop of experts to develop improved evaluation methods. The goal is to eventually communicate CMAQ strengths and shortcomings to the community and clearly define the limits of the model's capabilities. We also recommend formal model comparisons using a wide range of available models and chemical mechanisms. Analysis should utilize high time resolution data for ozone, other species and meteorological variables. Continue to work with ozonesondes and other vertical data. Evaluations should emphasize the use of process analysis type comparisons.

Model response analysis (Priority High)

Intensify evaluation of CMAQ response to changes in emissions and meteorology. The response of ozone, HNO_3 and particle formation to NO_x emission changes resulting from the NO_x SIP is an excellent example of a dynamic evaluation. Other opportunities for dynamic evaluation of CMAQ should also be identified. When CMAQ is applied to model control strategy impacts, predict future air quality conditions, or many other applications, its performance in simulating pollutant *responsiveness* to emissions changes can be even more important than simulating pollutant concentrations. Thus, dynamic evaluation of the CMAQ model, examining how well it captures pollutant responsiveness to emissions changes, is crucial. Unfortunately, dynamic evaluation is both more difficult to conduct than operational evaluation, since responsiveness cannot be directly evaluated against observations and it appears to have received short shrift relative to the other forms.

EPA has taken an important first step in dynamic evaluation by examining how well CMAQ captures the impacts of the NO_x SIP Call. More should be done to pursue the NO_x SIP Call research in greater depth, especially since the initial findings suggest that CMAQ may be underpredicting ozone responsiveness to NO_x emissions and/or meteorology. EPA should also identify other opportunities (e.g., Clean Air Interstate Rule, Clean Air Mercury Rule, diesel policies) for conducting dynamic evaluation of CMAQ, including cases that go beyond the NO_x -ozone relationship to also consider particulate matter or mercury. Dynamic evaluation should be linked where possible with diagnostic evaluation to examine why responsiveness is either over-predicted or under-predicted. It is our hope that less frequent releases of CMAQ may alleviate

some of the burden on operational evaluation and free up time for more in-depth dynamic and diagnostic evaluations.

Protocol for model performance evaluation (Priority Medium)

State environmental agencies are tasked with developing models for SIP attainment. What is missing in the current guidance is a protocol for a rigorous process based performance evaluation of these models. In practice, a typical model performance evaluation consists of statistical measures of output concentrations and eight-hour averages. These metrics may hide compensating errors that permit the model to match observed concentrations. AMD should play a key role in developing a protocol that emphasizes model performance evaluations based on whether the model achieved the right pollutant concentrations for the right reasons.

Assimilation of GOES cloud fields

AMD should consider directly assimilating the GOES cloud fields into MM5 by nudging the cloud liquid water field.

4-4. Charge Question 4: *What are your perceptions of the integration across different elements of the CMAQ Modeling Program (links between model development, applications, evaluation)? What is your perception of the usefulness of the CMAQ Modeling Program to the EPA, states, other customer needs and research community?*

In general the CMAQ Program has done an excellent job in integrating its efforts, with Division scientists in frequent communication and collaboration with each other. It is vital to develop and maintain two-way communication with the AQ research and applications communities. Periodic reviews are an excellent way to get input from a sub-set of the research community. But the CMAQ team at EPA is in a unique position to also identify present shortcomings of the modeling system, especially now that it is being run in a forecasting mode. Communicating these shortcomings and the areas of greatest need for further research, can focus the outside research communities efforts to better help in improving the model. For example it is important to interface with field programs. AMD should help frame research questions from a CMAQ perspective.

The CMAQ Program does an outstanding job of serving the needs of other EPA divisions and is relied upon by the many states who apply CMAQ for SIP development. The annual CMAS Workshop has served as a vital forum for EPA scientists to present their work to and interact with regulatory and research community modelers who use CMAQ. We encourage CMAQ and CMAS to set up a more formal survey of the users and other stakeholders to identify their needs and concerns. They need to perform a formal exercise of identifying what are the main issues, what can best be addressed and what will affect the users most positively.

The time between CMAQ releases should be lengthened, perhaps to 18 or 24 months. This would free up more of Division scientists' time to be devoted to improving the model and dynamic and diagnostic evaluations, because less time would be spent coordinating releases and version-by-version operational evaluations.

4-5. Charge Question 5: *Are there modeling research areas that are not being addressed or are given insufficient attention within the CMAQ Modeling Program? Are there current areas of research emphasis that might be given lower priority or eliminated? For the resources available to the CMAQ Modeling Program, are they being used in an effective manner in terms of the choice and quality of research being conducted?*

Overall, AMD is using its resources in a highly effective manner. The allocation of effort among model development, application and evaluation is good. However, the frequent releases of CMAQ mean considerable resources are spent assembling each year's version of CMAQ and on operational evaluations comparing that version with the previous release. Less frequent releases may free up resources for other efforts. EPA is on track in prioritizing improvement of the SOA module for its next release of CMAQ. While important improvements have been made recently or are forthcoming for vertical diffusion and cloud processes in CMAQ, it is not clear how much would be gained by further major efforts to improve transport processes until warranted by new developments in the literature.

In the Second Peer Review AMD presented a dramatic increase in the computational efficiency of CMAQ. Improvement in overall computational efficiency is very important to RPOs and state and local governments. Numerics were not greatly addressed during this review. The panel suggests that this is one area that should be addressed over the next 1.5 years. Increasing the computational efficiency of CMAQ, cleaning up some parts of the code, making it more robust (e.g., rechecking mass conservation issues and greater efforts in insuring the portability to new computational environments, etc.) should be a high priority.

Ensemble forecasting and the two-way interaction between WRF and CMAQ are two issues that are not very relevant to regulatory application but are potentially very important to the air quality forecasts. Historically, the chemistry component of air quality models has been run independent of the meteorological component. As a consequence, changes to the chemical concentrations have had no effect on the meteorology. In particular, aerosol concentrations have had no effect on radiative transfer and also have not influenced cloud microphysics. To fully include interactive chemistry and meteorology requires the passing of information between the chemical and meteorological models at frequent time intervals. Tests using MM5 (as well as WRF-Chem) have shown that two-way coupling can have a non-trivial impact on surface radiation (up to 25 W/m²) and on vertical mixing within the PBL. AMD has developed a plan to create two-way coupling between CMAQ and the WRF meteorological model, in which CMAQ is called as a subroutine of WRF.

This direction entails a considerable amount of effort. A primary advantage of retaining a separate chemistry module with the option of 1 or 2-way coupling with a meteorology model is that of flexibility. This will allow for model intercomparison studies where uncertainties associated with meteorological model uncertainties can be better evaluated. This option will also allow for multi-model ensemble forecasting. However, because the chemistry and meteorological components maintain distinct identities in the WRF-CMAQ framework, some of the meteorological fields are recomputed within the chemistry model, with a potential danger of introducing inconsistencies between two components. Sources of such inconsistencies should be

clearly identified and efforts should be made to reduce them and account for any remaining ones during the model evaluation stage.

Although AMD did not specify a time frame, the implementation of this plan is essential if CMAQ is to maintain the same capabilities as WRF-Chem and we hope that the two-way coupling will soon become available in a WRF release. Related to two-way coupling, efforts should address as to whether the present CMAQ mass-conservation scheme is adequate, particularly in regions of complex terrain or when convective clouds are present. Does on-line coupling within the WRF framework provide any real advantages for mass conservation? Will this be also true for other meteorological model choices – MM5, RAMS, MC2 etc.? It will be also of interest to explore avenues of coupling WRF and CMAQ where the structure may be more modular as opposed to the CMAQ being called as subroutine of WRF. The earth system modeling framework approach may also be explored.

Model reforecasting is the process of using a long time-series of model forecasts to remove seasonally or flow-regime dependent biases in the model, in a way similar to MOS-type corrections. It has recently come to be recognized as a very powerful tool that can significantly improve meteorological model skill. It is also particularly useful with an ensemble forecast system. We believe that reforecasting is something that AMD should consider in the mid-term future (2-3 years out) for its real-time AQ forecasts.

The use of ensembles in AQ forecasting offers great promise for improving predictive skill. However, the CMAQ group should do more to take advantage of already existing knowledge and tools regarding ensembles and work collaboratively with existing ensemble research programs within both the meteorological and air quality communities. For example, NCEP is funding university groups to work on air quality ensembles and other air quality forecasting developmental research and it would seem beneficial for the AMD air quality forecasting to be carried out in collaboration with these groups.

EPA should reconsider its approach to uncertainty modeling to ensure that a prudent approach is in place. The panel did not see sufficient evidence that EPA has developed a thorough strategy for examining model uncertainty or a plan for how this examination will inform other model development and evaluation efforts. The ensemble modeling conducted to date captures only a very narrow range of possible model set-ups (choices of MM5 set-up and chemical mechanism) and thus does not represent the full range of uncertainty in CMAQ. Past studies have shown that emission rates and, to a lesser extent, chemical rate constants are among the leading sources of uncertainty. Because many CMAQ applications depend as much on pollutant responsiveness as pollutant concentrations, any uncertainty analysis should identify uncertain parameters or other input choices most engendering uncertainty in responsiveness, not just concentrations.

5. COMMENTS ON THE PEER REVIEW PROCESS

We believe that the external peer review process for CMAQ is well conceived. We continue to believe that the highest reasonable frequency for reviews should be once every 18 months to two years. It is appropriate that the reviews alternate between broadly based and focused reviews.

The size and composition of the review panel with seven members was well balanced. Continuity of panel deliberations and coherence between reports was aided by the presence of two previous panel members. The package of relevant publications to review prior to the meeting and the electronic copy of all presentations greatly assisted the review. The third review followed a schedule that was similar to the second review. The schedule allowed sufficient opportunity for panel members to interact with AMD staff and the schedule was near optimal. We recommend that future reviews continue to employ a similar schedule. The reporting process for the Second Review was limited to a single iteration between the committee and CMAS/AMD and this helped to produce a high quality report within a reasonable time. We recommend that this limitation be continued in future reviews.

6. CONCLUSIONS

AMD staff working on the CMAQ Modeling Program are conducting state-of-the-science model development and research whose overall breadth and quality is unmatched by any other group worldwide. Model developers have done an outstanding job of incorporating new science as it becomes available. CMAQ is an operational tool used in applied research, regulatory analysis and air quality forecasting. The addition of the new mission to support air quality forecasting has placed new requirements on the modeling team. AMD balances the timely release of improved versions against stability so that the model can be used as a regulatory tool. AMD has generally succeeded in its attempts to balance the demand for scientific completeness and rigor in the model with the need for computational efficiency. The panel finds that CMAQ modeling program provides air quality models that are of high caliber. The panel recognizes that there is a wide range in the level of scientific understanding of the processes modeled and therefore evaluation of CMAQ simulations is a continuing priority.

AMD continues to make significant progress since the last review (Amar et al., 2006). Major new developments to CMAQ include an updated carbon bond chemical mechanism, improvements to the heterogeneous chemistry, the treatment of aerosols by ISORROPIA, an increase in the numbers HAPS that can be modeled and the implementation of a new planetary boundary layer model, asymmetric convective model, version 2. Also there are a number of significant CMAQ improvements in progress including the development of a new secondary organic aerosol module, a new coarse particle chemistry module, an in-line photolysis module, implementation of the WRF/CHEM convective cloud model, methods to assimilate GOES derived clouds into CMAQ and methods for coupled synchronous meteorology and chemistry calculations.

The panel was delighted to learn that AMD was responsive to the second review panel's recommendations (Amar et al., 2006). The responses include a number of significant activities that are mentioned here. AMD staff have actively participated in the EPA/NERL post-doc program. Team members have worked more closely with the regulatory modeling community to obtain first-hand knowledge of how models are being applied and evaluated by these groups. They have worked to improve the treatment of the heterogeneous chemistry of N_2O_5 . AMD is working on the development of a sectional approach to provide an improved description of the aerosol size distribution. Treatment of the interactions between gases and coarse aerosols is being developed for ISORROPIA. SOA chemistry is being upgraded in accord with the panel's

recommendation. The re-emission of volatile and semi-volatile compounds will be treated in CMAQ. Sub-grid vertical transport in deep convection will be improved through the implementations of the Grell convective cloud parameterization scheme. The representation of vegetation between BEIS and deposition models is being improved.

More intensive measurements from field studies are being sought to supplement the weak measurement base for evaluation of CMAQ-Hg. Work is in progress to examine the possibility of coupling the regional CMAQ model with global chemical transport models. Dynamic evaluation is now one of AMD's focus areas in model evaluation to better link model response to changes in emissions. AMD is working to improve the characterization of clouds and precipitation.

The panel finds that the Atmospheric Model Evaluation Tool (AMET) project should have a high priority. It is desirable that AMET's functionality will be expanded to also include satellite derived fields and other non-standard data sources. AMET should be adapted to accommodate ensemble based modeling. AMT should also develop methods to allow users to incorporate new analysis tools into AMET. The panel rated the transition to WRF, improving cloud chemistry and physics including the aqueous phase, SOA formation and mechanism performance evaluation and the quantification of uncertainty in pollutant predictions as high priorities. The panel rated the improvement of the aromatic chemistry mechanism, assessment of the uncertainty in dry deposition and multimedia modeling as medium priorities. Low priority activities that could go forward only as budget and staffing allows include HAP chemistry and fine-scale modeling and exposure. The weaknesses of the science being used in CMAQ components reflects weaknesses in current scientific understanding, including mercury chemistry, cloud processes and secondary organic aerosol formation. We also agree with future work suggested by the presenters, including the addition of the RACM2 chemical mechanism within CMAQ, inclusion of surface heterogeneous HONO source to improve model performance, the combining of gas and aqueous phase chemistry modules and the implementation of source apportionment tools for PM trace elements.

The panel commends AMD staff for their commitment to the continuing evaluation of CMAQ. The panel recommends that AMD convene a workshop of experts to develop improved evaluation methods. Formal model comparisons designed to communicate CMAQ strengths and shortcomings to the community for each application is a high priority. Another high priority for CMAQ is its' dynamic evaluation to evaluate its performance in simulating pollutant responsiveness to emissions changes. A medium priority is to provide an improved guidance document with an evaluation of its' performance and uncertainty for various applications. Midway between simulation and evaluation is improved data assimilation, for example, AMD should consider directly assimilating the GOES cloud fields into MM5 by nudging the cloud liquid water field.

The CMAQ development team has done an outstanding job of serving the EPA, the states, regional organizations and the scientific community. A more formal process to survey the users to identify their needs and concerns should be established. The time between CMAQ releases should be lengthened, perhaps to 18 or 24 months. This would free up more of their time to devote to other priorities.

Computational efficiency of CMAQ was not greatly addressed in this review in contrast to the Second Peer Review. The panel suggests that this is one area that should be given at least a medium priority over the next 1.5 years. The development of ensemble forecasting and the two-way interaction between WRF and CMAQ are high priority developments for improving air quality forecasting. Ensemble forecasting and two-way interaction may have utility for regulatory purposes but AMD needs to develop a very specific plan to develop this application. AMD needs to ensure that their ensemble modeling captures a much broader range of possible model configurations and run conditions, including emission rates. Also for air quality applications reforecasting should have a high priority.

In conclusion, the panel commends AMD for their excellence. Their presentations were of very high quality and clearly they are very competent researchers. The review panel was highly impressed their commitment to continue to make improvements to CMAQ, its' evaluation and applications. CMAQ represents the state-of-the-science in regional air quality models.

7. REFERENCES

Amar, P., R. Bornstein, H. Feldman, H. Jeffries, D. Steyn, R. Yamartino and Y. Zhang, 2004: *Final Report: December 2003 Peer Review of the CMAQ Model*. Report submitted to Community Modeling and Analysis System Center, University of North Carolina at Chapel Hill, July, 24 pp.

Amar, P., D. Chock, A. Hansen, M. Moran, A. Russell, D Steyn and W. Stockwell, 2005: *Final Report: Second Peer Review of the CMAQ Model*. Report submitted to Community Modeling and Analysis System Center, University of North Carolina at Chapel Hill, July, 33 pp.

Lee, S.; Kamens, R. M. " Particle Nucleation from the Reaction of alpha-Pinene and O₃" *Atmospheric Environment*, 39, 6822-6832, 2005.

Leungsakul, S.; Jeffries, H.E.; Kamens, R.M. "A Kinetic Mechanism for Predicting Secondary Aerosol Formation from the Reaction of d-limonene with NO_x and Natural Sunlight", *Atmospheric Environment* 39, 7063-7082 2005.

Leungsakul, S.; Jaoui, M.; Kamens, R. M. "A Kinetic Mechanism for Predicting Secondary Aerosol Formation from the Reaction of d-limonene with Ozone" *Environ. Sci. Technol.* 39, 9583-9594, 2005.

Tolocka, M. P.; Jang, M.; Ginter, J.M.; Cox, F.J.; Kamens, R.M.; Johnston, M.; "Formation of Oligomers in Secondary Organic Aerosol", *Environ. Sci. Technol.* 38, 1426-1434, 2004.

8. APPENDIX. CHARGE AND AGENDA FOR THIRD CMAQ PEER REVIEW MEETING

CHARGE TO CMAQ MODEL PEER REVIEWERS

The 2006 Peer Review will emphasize meteorological/physical/chemical process aspects of the CMAQ modeling program, as well as applications and evaluation. EPA=s program in air quality modeling within the Atmospheric Modeling Division (AMD) of the National Exposure Research Laboratory (NERL) *transitions research grade air quality models to operational tools* for use in policy and regulatory analyses. The CMAQ Model Program Peer Review Panel is charged with addressing the following questions regarding the quality and productivity of the applied research program within AMD, with emphasis on the aspects mentioned above, bearing in mind that the object of our research program is to develop air quality models for regulatory/operational purposes.

1. What is the overall quality of the applied scientific research in the CMAQ Modeling Program?
2. What are the strengths and weaknesses of the science being used within the components of the CMAQ Model development program?
3. What is the quality and relevance of the model applications and evaluations being conducted as part of the CMAQ Modeling Program?
4. What are your perceptions of the integration across different elements of the CMAQ Modeling Program (links between model development, applications, evaluation)? What is your perception of the usefulness of the CMAQ Modeling Program to the EPA, states, other customer needs and research community?
5. Are there modeling research areas that are relevant to the EPA=s regulatory program needs not being addressed or are given insufficient attention within the CMAQ Modeling Program? Are there current areas of research emphasis that might be given lower priority or eliminated? For the resources available to the CMAQ Modeling Program, are they being used in an effective manner in terms of the choice and quality of the applied research being conducted at AMD, NERL?

CMAQ PEER REVIEW MEETING
December 18-20, 2006
U.S. EPA – Research Triangle Park, NC
Conference Room C112

Agenda

December 18

8:30am	Introductions / Background / Charge to Reviewers	S.T. Rao
8:45am	Summary of May 2005 Peer Review Findings and EPA Response	K. Schere
9:15am	Overview of 2006 CMAQ Model System Release And Plans for 2007 Release	K. Schere
9:45am	BREAK	
	Meteorological Process Research and Modeling	
10:00am	1. Transition to WRF (P-X LSM, Nudging)	T. Otte
		J. Pleim
10:40am	2. Boundary Layer Modeling (ACM2)	J. Pleim
11:15am	3. MCIP/PREMAQ Development	T. Otte
11:45am	Emissions Estimation (fires, biogenics)	T. Pierce
12:15pm	WORKING LUNCH	
	CMAQ Processes	
1:30pm	1. Chemical Developments (CB05, air toxics, Cl, Hg)	G. Sarwar
2:15pm	2. Aerosol Developments (fine-coarse interactions, SOA, H2O2-het, ISORROPIA)	P. Bhawe
3:00pm	BREAK	
3:15pm	Fine-scale Modeling and Links with Human Exposure (hybrid modeling; CMAQ/HYSPLIT, etc.)	V. Isakov
3:45pm	Integrated Meteorology/Air Quality Modeling (WRF-CMAQ; WRF-Chem; ESMF)	J. Pleim
4:45pm	Discussion Period	
5:15pm	END OF FIRST DAY	

December 19

8:30am	CMAQ Model Applications - Introduction	R. Dennis
	Deposition Processes and Multimedia Modeling	
8:40am	1. Multimedia modeling applications and evaluation	R. Dennis
9:30am	2. Dry deposition process modeling in CMAQ	D. Schwede
10:00am	3. Wet deposition process modeling in CMAQ	S. Roselle
10:30am	BREAK	
11:00am	Air Quality Forecasting – What have we learned to improve AQ modeling?	R. Mathur
12:00pm	WORKING LUNCH	
	CMAQ Model Evaluation – New Directions	
1:30pm	1. Overview	A. Gilliland
2:15pm	2. Evaluating CMAQ's ability to represent air quality responses to emission changes – Dynamic Evaluation	A. Gilliland
2:45pm	BREAK	
3:00pm	3. Meteorological Model Evaluation and Impacts on Air Quality	R. Gilliam
3:30pm	4. Considering model uncertainty in evaluation and application of CMAQ	R. Pinder
4:00pm	Discussion Period	
4:45pm	Wrap-up Comments	K. Schere
5:00pm	END OF SECOND DAY	

December 20

8:30am	Small group or one-on-one discussions between Peer Reviewers and CMAQ scientists
10:00am	Panel Deliberations and work time
11:00pm	Debriefing to AMD Management and PIs
12:00pm	END OF PEER REVIEW MEETING